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IMAGE ANALYSIS USING QUANTUM ENTROPY, SCALE SPACE AND DIFFUSION CONCEPTS

Colorado School of Mines

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14. ABSTRACT

This report documents investigations of the connections between scale space and the linear and nonlinear diffusion of images, as well as investigations of concepts of generalized entropy and quantum entropy and their measures. The generalized entropies included in particular Renyi entropy with parameter q. The diffusion studies were performed with a combination of mathematical analysis and simulations. Analysis of quantum and semi-classical entropies of modeled physical systems was also performed. The feasibility of applying forms of generalized quantum search to scheduling and logistics problems was also investigated. As part of this effort, simulations of adaptive quantum search were performed. Furthermore, the capabilities and constraints of quantum lattice gas algorithms (QLGAs) were investigated, and a new QLGA for the telegraph equation with one spatial dimension was formulated, implemented, and simulated.

15. SUBJECT TERMS

image processing, entropy, diffusion, scale space, quantum lattice gas algorithm, logistics problems, quantum adaptive search

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1. Overview and Project Goals

Our research investigated the connections between scale space and the linear and nonlinear diffusion of images using a combination of analytic methods and prototype Matlab and Mathematica programs. We investigated concepts of generalized entropy and quantum entropy and their measures, using mathematical analysis. The generalized entropies included in particular Renyi entropy [renyi] with parameter q. We also examined the properties of generalized entropy of images subject to linear and nonlinear diffusion processes. We performed analysis of quantum and semi-classical entropies of model physical systems.

We investigated the feasibility of applying forms of generalized quantum search to scheduling and logistics problems. As part of this effort, we performed simulations of adaptive quantum search. Based upon this portion of the research, Ben J. Jones received the Ryan Sayers memorial award for research as a senior student majoring in both computer science and engineering physics.

As a further goal, we investigated the capabilities and constraints of quantum lattice gas algorithms (QLGAs), including the properties of their (unitary) collision operators. QLGAs are known to be able to simulate a variety of partial differential equations [yepez], including the Navier-Stokes, Boltzmann, and Dirac equations [iwoprd]. In our research, we investigated the feasibility of the solution of the celebrated Maxwell equations of electromagnetism by means of QLGAs [coffey]. We also formulated, implemented, and simulated a QLGA for the telegraph equation with one spatial dimension [cc2009]. The latter equation combines facets of both the wave and diffusion equations. Our research indicated that the simulation of the 1D linear telegraph equation with an iterate constraint has application to signal denoising.

2. Approach

Consideration of classical and quantum entropy and their application motivated much of our initial effort. Furthermore, entropy concepts occurred throughout much of the later research. Most explicitly they appear in the consideration of image entropy, but also later for instance in the Schmidt strength from quantum logic gate decomposition. This form of entropy gives a measure of the nonlocal content of an entangling logic gate.

Entropy and its generalizations are among the most important measures of information content and complexity of signals and images. Another important concept that we made use of was that of scale spaces. In scale-space theory one embeds an image into a continuous family of gradually smoother versions of it. The time t acts as a parameter for this, with the original image corresponding to t = 0. Increasing the scale should simplify the image without creating spurious structures. For instance, in viewing a facial image at coarser scales, it would be undesirable to have artificial features appearing. A scale-space introduces a hierarchy of image features, and can provide an important process in going from a pixel-level description to a semantical image description.

Partial differential equations (PDEs) are the suitable framework for scale-spaces, and the oldest, simplest, and probably most studied version of scale space corresponds to a linear diffusion process. The fundamental solution (Greens function) for a linear heat or diffusion equation is a Gaussian function with standard deviation proportional to the square root of the time. The solution of the linear diffusion equation can be given as the convolution of the initial data (image) with this Gaussian function, and this gives linear scale space. For the extension to nonlinear scale space, the PDE involved is a nonlinear diffusion equation with a decreasing diffusion coefficient D. When D depends upon the magnitude of the gradient of the pixel intensities, we generally obtain selective smoothing. Locations where the gradient is large have strong probability of being an edge, and D is reduced.

A form of the diffusion (or heat) equation is $\partial I/\partial t = \nabla \cdot [D(I) \cdot \nabla I]$, where I is the image intensity. For linear and isotropic diffusion in two dimensions, the diffusion equation is simply $I_t = D(I_{xx}+I_{yy})$. The basic idea of anisotropic diffusion is to diffuse intensities along edges of objects that appear within an image, while not diffusing (or even enhancing the contrast) along directions that are perpendicular to edges [perona, price]. For nonlinear diffusion of images to generate intraregion smoothing, $D = D(|\nabla I|)$, and regions of high intensity contrast undergo less diffusion.

The diffusion boundary value problem is completed with the specification of initial and boundary conditions. The initial condition is simply $I(x,y,t=0) = f(x,y)$, where f is the given image. Homogeneous Neumann or periodic boundary conditions are appropriate as they lead to conservation of the average grey values of the whole image. This fact results from the divergence form of the diffusion equation.

In the mathematical sense, the partial differential equations we simulated with QLGAs are evolution equations of the form

$$u_t = f(u,u_x,u_{xx}), \tag{1}$$

where the subscripts denote partial differentiation, for example, $u_t \equiv \partial u/\partial t$. Therefore, we solved equations that are first order in time and second order in space. The PDE is supplemented by an initial condition $u(x,t = 0) = u(x,0)$ and boundary conditions at the endpoints of the x-interval to completely specify the problem. We used most often periodic boundary conditions, so that for a one-dimensional problem on an interval of length L, $u(0,t) = u(L,t)$. For image processing applications in particular, the dependent variable u corresponds to pixel intensities. For heat transfer problems, u represents the temperature, while for fluid flow problems u corresponds to either the mass density or flow velocity.

A quantum lattice gas algorithm is a quantum version of a classical lattice gas, which in turn is an extension of classical cellular automata [yepez, doolen]. In place of the binary lattice variables of a classical lattice gas, the quantum version has a local Hilbert space describing the quantum bit (qubits). In the classical case, in order to recover the proper macroscopic dynamics (and thermodynamics), it is important to ensure that the microscopic dynamics preserves conservation laws. Similarly, in the quantum case, the number densities of qubits must be preserved so that the interaction operator, called the collision operator, must be unitary.

The operation of a type-II quantum processor includes the sequential repetition of four main steps [berman, yepez, vahala, love]. First, initialization creates the quantum-mechanical initial state that corresponds to the initial probability distribution for a partial differential equation to be solved. Secondly, a unitary transformation (collision operator) is applied in parallel to all the local Hilbert spaces in the lattice. Next, in the measurement step, the quantum states of all the nodes are read out. Lastly, these results are streamed to neighboring sites to reinitialize the quantum processor in the state which corresponds to the new probability distribution.

After the initialization step, a quantum lattice gas algorithm performs iterations of a collision operator and a streaming operator. The latter operator shifts the state of a qubit from a given lattice site to its nearest neighbors in the lattice.

3. Details of Technical Accomplishments

3.1 Entropy investigation

3.1.1 Diffusion processing

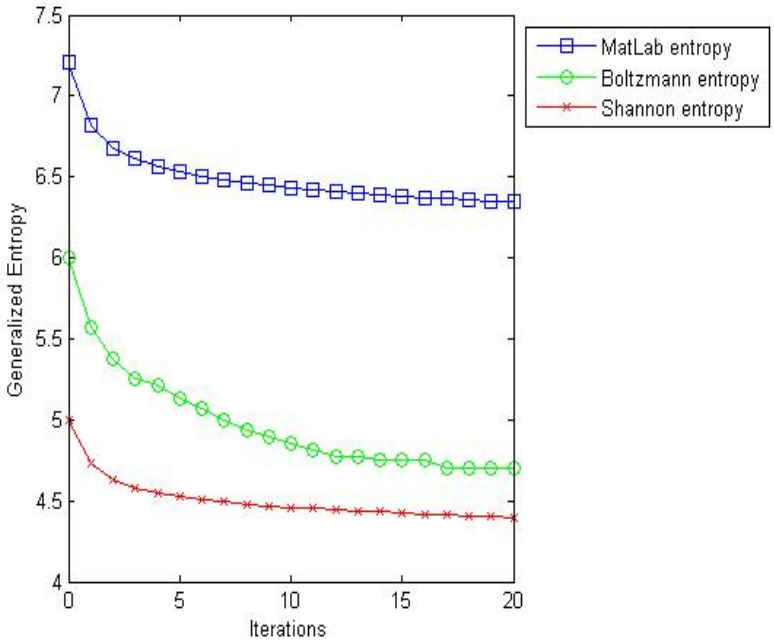
Diffusion processing has proven very useful for practical image enhancement, wherein the visual quality of an image is improved. We have investigated methods of carrying out such processing in a combined classical-quantum computing environment.

We performed investigations specifically examining the change in generalized entropies, including Renyi entropy [renyi]. We are motivated to examine the Renyi entropy because it seems to comport well with the ideas of scale spaces discussed above. Like Tsallis entropy, Renyi entropy contains a parameter $q \neq 1$: $S_q(p) = \ln[\Sigma_{j=1}^{N} p_j^q]/(1-q)$, where p_j are normalized pixel values. It also reduces to the Shannon-Wiener entropy when $q \rightarrow 1$: $S_{SW}(p) = -\Sigma_{j=1}^{N} p_j \ln p_j$. Here we have sums over pixel values (probabilities) since we are in the discrete (digital) case rather than integrals suitable to the continuous case. We see that the Renyi entropy gives a sort of extrapolation of the Shannon-Wiener entropy [karolz]. The parameter q serves to introduce a type of weighting of pixel values into the entropy and may help to provide a hierarchical ordering of the image information. Therefore, it is directly connected to scale spaces.

Figure 1 shows an example of the decrease of various entropies upon successive iterations of nonlinear diffusion with an exponential diffusivity function. The image entropies are determined from the histogram of the distribution of pixel intensities. Matlab's entropy just uses a different base (2) of logarithm than Shannon. The change in image entropy during diffusion processing is a reflection of the loss of information in going from finer to coarser scales of resolution.

We may list the following as desirable properties of entropy as applied to image processing tasks. These points could serve as guidelines for future research (cf. [starck]), or as a start on axioms for developing measures of information content.

- A single-value image has zero information content.
- The amount of information in an image is independent of the background.
- The amount of information is dependent on the noise.
- The entropy should work in the same way for a pixel that has value $V + \delta$ and for a pixel with value $V - \delta$, with V being the background value.
- The amount of information is dependent on the spatial correlation in the image. An image with large homogeneous features (above the noise) contains less information.



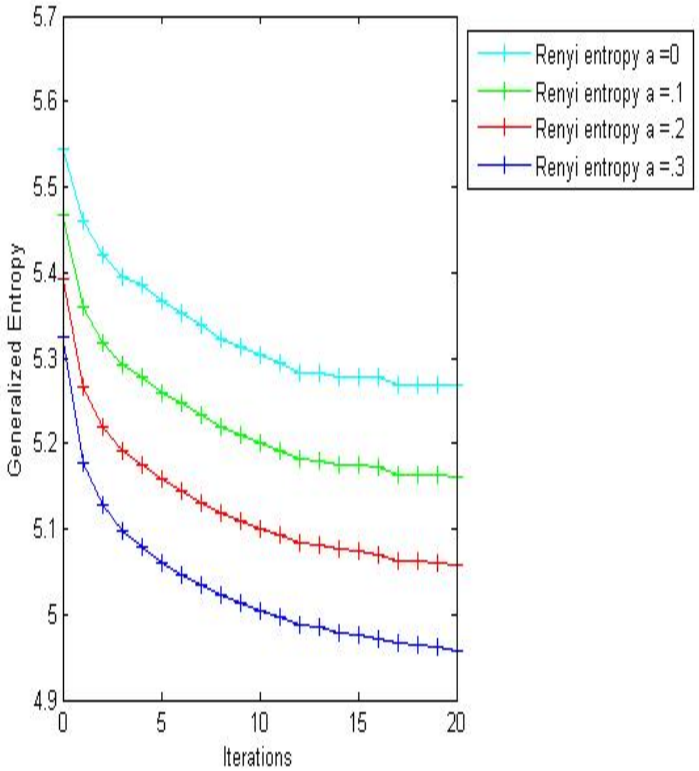


Figure 1. Decrease of generalized image entropy with iteration number during nonlinear diffusion processing.

3.1.2 Entropy calculations for model physical systems

Lately information theoretic concepts have been playing a larger role in quantum mechanics and quantum computing. Information concepts have been employed in both fundamental discussions and in practical applications including synthesis and analysis of electron densities in position and momentum space [gadre]. Indeed, the sum of quantum position and momentum entropies has been advocated as a measure of wavefunction quality [gadre].

Quantum entropy provides a quantitative description about the uncertainty or lack of knowledge of an observable. For instance, the entropy is one measure of the delocalization of a wavepacket. The Shannon entropy provides an unambiguous measure which is complementary to the information content of a system. With the recent research into quantum computing [kitaev, nielsen, qcreviews] there has been added attention on the fundamental physical limits of computation [cofpla] and here also the quantum entropy plays a role.

We recall that Hirschman [hirschman] anticipated a strengthened quantum uncertainty principle. Later, Deutsch [deutsch] and others [bbm] showed that the Heisenberg inequality does not properly express the quantum uncertainty principle and is generally too weak. They introduced entropy measures such as we use for noncommuting observables.

In [coffeycjp] we established the semiclassical position and momentum information entropies for a family of systems with rational potential energies and for the sech^2 potential energy. The latter is an important instance since it applies to a potential with nonpolynomial form. It also includes the case of an attractive delta-function potential for certain limit values of the potential parameters of strength and width. The resulting semiclassical entropy relations have high utility. This is because otherwise numerical computation may be required, or when closed form results for quantum systems are available, the multiple sum and product expressions do not readily yield physical information.

A further motivation of our investigation was a recent presentation of the ground state position entropy of the Poeschl-Teller potential [atre]. The hyperbolic form of this potential is none other than the sech^2 functional dependence that we employ. The study [atre] gave some numerical results for excited states, although we note that the exact general excited state solution is expressible in terms of products of operators $O_p = d/dx - p \tanh \alpha x$ [lamb]. Since asymptotic relations are now known connecting quantum entropies to classical counterparts for both position [ruiz] and momentum [cofmomentum], we are able to derive semiclassical expressions applicable for high excited states.

The entropic uncertainty relation gives a lower bound to the sum of position $S^{(x)}$ and momentum $S^{(p)}$ entropies [bbm],

$$S_Q^{(x)} + S_Q^{(p)} \geq D(1 + \ln \pi), \tag{2}$$

for a D-dimensional system. This inequality stresses the reciprocity of position and momentum spaces. For if the wave function is concentrated in coordinate space, it will necessarily be more diffuse in momentum space, and vice versa. Not surprisingly, the bound in Equation 2 is attained by Gaussian wave functions [bbm]. Relation 2 extends to other pairs of noncommuting observables A and B, $S^{(A)} + S^{(B)} \geq s_{AB}$, where s_{AB} is a positive constant. From Equation 2 follows the Heisenberg uncertainty relation, showing that this inequality is stronger.

The entropy sum appears in many other lower and upper bounds. Another lower bound including measurement device resolutions Δx of position and Δp_x of momentum is [bbirula]

$$S_Q^{(x)} + S_Q^{(p)} \geq 1 - \ln 2 - \ln \Delta x \, \Delta p_x. \tag{3}$$

An upper bound to the entropy sum can be prescribed in terms of the second moments in position and momentum space [gadre]. We note that the entropic uncertainty relation has been extended to nonzero temperatures T [abesuzuki].

In the case of the sech^2 potential we recall that the classical period of motion depends upon total energy E as $T(E) \sim |E|^{-1/2}$. We then determine how the classical position entropy $S_C^{(x)}$ varies logarithmically with the energy. By invoking an asymptotic relation [ruiz], we then know how the quantum entropy of position $S_Q^{(x)}$ varies for the nth energy eigenstate. Since we also know the values of the energy levels E_n, we determine explicitly the dependence of the semiclassical position entropy upon principle quantum number n. We find the momentum entropy $S_C^{(p)}$, and therefore $S_Q^{(p)}$ for highly excited states [cofmomentum], to contain $\ln |E|^{-1/2}$ dependence, which is not surprising given that the Hamiltonian is quadratic in momentum p. In the paper [coffeycjp] all these relations are made quantitative. The calculations require fairly advanced integration techniques. In particular, we extended several known results employing the Gauss hypergeometric function.

Semiclassical results are also possible and discussed for a family of rational potentials in [coffeycjp]. The treatment of this set of potentials also relies heavily upon the analytic properties of the hypergeometric function. This family contains a parameter q, $V(x) = -V_0/[1+(|x|/a)^q]$, where $V_0 > 0$, such that the limit $q \to \infty$ yields the finite square well as shown in Figure 2. For q = 2 the rational potential is very similar to the sech^2 potential about the common minimum at x = 0.

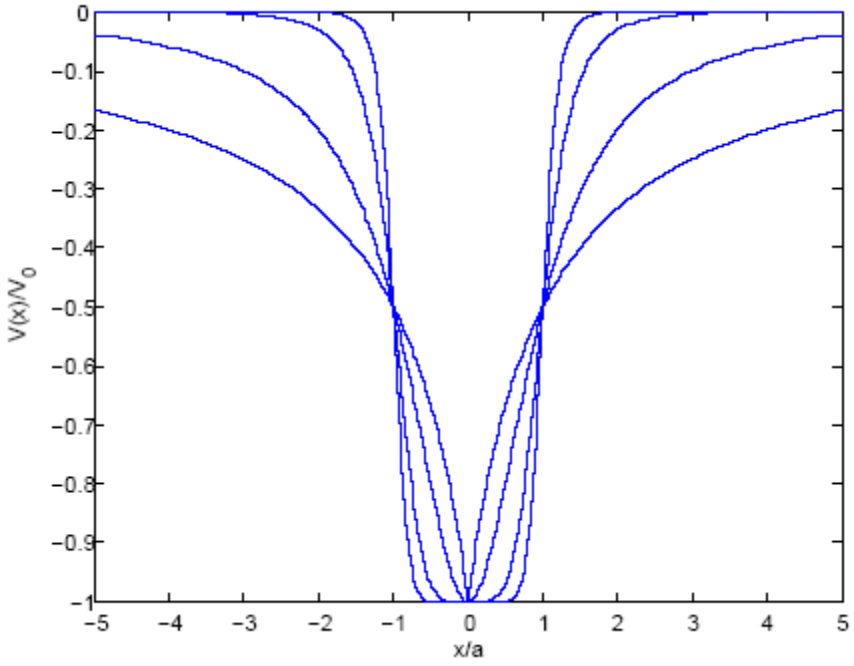


Figure 2. The sequence of potentials $V(x)/V_0 = -1/[1+(|x|/a)^q]$ obtained for varying values of q is plotted versus x/a.

3.2 New quantum algorithm for the modal value

In this section we present a quantum algorithm for finding the most often occurring (or modal) value of a data set. We thereby supplement other algorithms that can determine the mean value or similar quantities. Our algorithm requires the combined use of quantum counting and extended quantum search.

The mode is the most often occurring value in a data set and is an important statistic. For the sake of definiteness in the description, we assume a data list of N elements, each entry being an integer in the range [1,d]. We propose an algorithm that uses a combination of quantum counting [brassard] and quantum search [boyer, grover1, grover2, grover3, nielsen], and makes use of the result that quantum search may be applied to find more than one target item in an unsorted list and that the number of target items need not be known beforehand. Our method gives an operational complexity of $O(d\sqrt{N})$, as measured in the number of oracle calls. The modal value need not be unique for our algorithm to succeed.

Our algorithm for determining the mode is related to other algorithms that also apply quantum search, give a quadratic speed up over the classical situation, and deliver other useful statistics. These include an algorithm for finding the minimum or maximum value in a data set [durr]. In addition, the mean value may be determined by [grover2], and then the variance and higher moments of a data set may be determined. This is because the moments may be appropriately written as averages. In particular, the variance is the mean value of the quantity $(x-\langle x\rangle)^2$, where $\langle x\rangle$ is the mean value. The median value may also be estimated, with an algorithm giving a nearly quadratic speed up over classical algorithms in the worst case [nayakwu].

Because of the utility to compute averages, quantum search also has application to integration. On the other hand, we are interested to have quantum algorithms to determine a large variety of statistics of given data. Such statistics could be used for instance in analyzing digital images by applying them to the pixel intensities. Operations such as thresholding and region segmentation or dilation and erosion could be performed based upon the statistical values.

We recall that quantum counting relies on phase estimation and the Fourier transform. Quantum counting exploits the periodicity with the number of Grover iterates of the probability amplitude of the target state(s). In turn, quantum phase estimation makes use of controlled-U^{2j} operations and the inverse Fourier transform to give the best n-bit estimate of the phase ϕ of the eigenvalue $e^{i\phi}$ of the unitary operator U.

The quantum search algorithm has been extended in a number of ways, including with different iteration operators and different selective phase shifts (e.g., [biham, galindo, grover2]). These are implementation specific matters that are not the focus of this discussion.

3.2.1 The algorithm

For simplicity of description, we assume that no value, including specifically the modal value, occurs more than N/2 times in the data set. This is not a limitation, since if this number $M \geq N/2$, the number of items in the data set may be doubled with N non-solution elements, and a modified oracle for quantum search may be suitably constructed [nielsen].

We assume that the data values are bounded by the range [1,d]. We consider two quantum registers $|D\rangle$ and $|C\rangle$, the data and count registers, of size $O(\log_2 N)$ and $O(\log_2 d)$ qubits respectively. The algorithm has two main steps.

First, we initialize the quantum system as $|D\rangle|0\rangle$. Then for each data value in the first register we use quantum counting [brassard] to determine if that value occurs and if so how many times, such count being kept in the second register. We then apply the quantum algorithm for determining the maximum value [durr] that uses the generalized quantum search algorithm [boyer] to the $|C\rangle$ register. This returns the number of times M the modal value occurs.

Secondly, we reinitialize the system as $|D\rangle|0\rangle$. We then execute an extended quantum search to find the data element(s) corresponding to the previously determined number of times that the modal value occurs. In this case, the oracle function indicates which target item(s) occurs M times.

This algorithm delivers both M and the corresponding modal value(s) of the data set. By the use of extended quantum search, the modal value need not be unique.

3.2.2 Discussion and Summary

The probability of success of our algorithm can be boosted to be arbitrarily close to 1 throughout. Suppose we desire a small probability of failure $1 >> \varepsilon > 0$. To guarantee that all of our counting operations succeed with probability of at least $1-\delta$, we require complexity $O(d\sqrt{N}\log(d/\delta))$. This gives our algorithm total probability $\geq (1/2)(1-\delta)$ of success [furrow]. From here we appeal to amplitude amplification [bcwz] for maximum finding, which leads to an overall running time of $O(d\sqrt{N}\log(d/\varepsilon)\sqrt{\log(1/\varepsilon}\}$, where ε is our total probability of failure.

Our work serves to enlarge the collection of quantum algorithms for determining statistics of a data set to include the modal value. A combination of both quantum counting and quantum search is required in order to avoid reducing to a classical O(N) complexity. Our description here is not intended to be exhaustive and it seems likely that several variations on the ideas presented are possible.

3.3 Quantum logic gate decomposition

Here we consider two-qubit operators and provide a correspondence between their Schmidt number and controlled-NOT (CNOT) complexity, where the CNOT complexity is up to local unitary operations. The results are obtained by complementary means, and a number of examples are given. For full details, see [coffeydeiotte].

An operator Q acting on systems A and B may be written as the operator-Schmidt decomposition

$$Q = \Sigma_j \, s_j \, A_j \otimes B_j, \tag{4}$$

where $s_j \geq 0$ and A_j and B_j are orthonormal operator bases for A and B, respectively. This form may be proved constructively by using the singular value decomposition. Given the representation (4), the Schmidt number Sch(Q) of the operator Q is defined as the number of nonzero coefficients s_j.

In this discussion we are concerned with two-qubit operators, and the relation of their Schmidt number to their controlled-NOT complexity. It is known that two-qubit unitaries are equivalent to either 0, 1, 2, or 3 CNOT gates, where the equivalence is up to single-qubit rotations (e.g., [makhlin02]). On the other hand, two-qubit unitary operators may have Schmidt numbers 1, 2, and 4, but not 3 [nielsenetal03]. (A similar result for states has been obtained in [dur02].)

We recall that the Schmidt number is an indicator of entanglement, but not a measure of entanglement. For instance, let us compare the Bell state

$$|\phi\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle),$$

with the state

$$|\psi\rangle = \sqrt{(1-\varepsilon^2)}|00\rangle + \varepsilon|11\rangle,$$

where we take $\varepsilon << 1$. Both of these states have Schmidt number two, but the Bell state is much more entangled, in fact maximally entangled. This simple example reflects a more general situation where a single term dominates in the Schmidt decomposition. The state is entangled, but it may be weakly so.

In [coffeydeiotte] we provide a classification of CNOT complexity viz a viz the operator-Schmidt decomposition, and prove it in alternative ways. We then provide several examples, and discuss related topics. Among these, we present relations between different approaches for finding the parameters of the canonical decomposition of two-qubit operators.

One may expect that as the Schmidt number increases, so too does the CNOT complexity. The main result is the following [coffeydeiotte]. *Proposition*: A two-qubit operator U with CNOT complexity 2 or 3 has Sch(U) = 4, with CNOT complexity 1 or 2 has Sch(U) = 2, and with CNOT complexity 0 has Sch(U) = 1.

Having considered CNOT complexity in relation to Schmidt number for two-qubit operators, an alternative way to express our classification is in terms of the Hartley strength, $K_{Har}(Q) \equiv \log_2[Sch(Q)]$. We find that $K_{Har}(U) = 2$ for operators U of CNOT complexity 2 or 3, $K_{Har}(U) = 1$ for those operators with CNOT complexity 1 or 2, and finally $K_{Har}(U) = 0$ for local unitaries. Among examples, the particular swap operation u_s and CNOT itself have $K_{Har} = 1$. The $SWAP^{\alpha}$ gate, with $0 < \alpha \leq 1$, as well as F, the quantum Fourier transform on two qubits, have $K_{Har} = 2$ and CNOT complexity 3. The classification that we have given is hierarchical, in the sense that operators of higher CNOT complexity or Schmidt number may simulate those of lower complexity, but not the other way around.

We have discussed alternative means for obtaining both the CNOT complexity of a two-qubit operator and its canonical decomposition [coffeydeiotte, cts]. Besides the operational decompositions given elsewhere, we have illustrated the constructive procedure of Childs et al. [childs] for finding the three nonlocal parameters of a canonical decomposition.

The operator Schmidt decomposition has with it a normalization that is convenient for probability and entropy considerations. For unitaries acting on systems A and B of dimensions d_A and d_B, respectively, the relation $tr(U^tU)=d_Ad_B$ gives that the Schmidt coefficients s_j satisfy $\Sigma_j\ s_j^2 = d_Ad_B$. Thus, the normalized coefficients s_j^2/d_Ad_B form a probability distribution. For the two-qubit operators U considered here, simply the numbers $s_j^2/4$ give a probability distribution. The Schmidt strength may be defined as the Shannon entropy of this distribution, providing a measure of the nonlocal content of U.

3.4 Scheduling and logistics problems via adaptive quantum search

The recent developments in the field of quantum computing have allowed computer scientists and others to view optimization problems from a new perspective. By framing optimization as a problem of unordered database search, these problems can be solved using algorithms based on Grover's quantum search, theoretically providing quadratic speedup in runtime. In 1996 Grover [grover, grover1, grover2, grover3] used the property of quantum parallelism to design an algorithm to search an unordered database in $O(\sqrt{N})$ time, a problem that classically takes O(N) time where N is the database size. It has been hypothesized that Grover's results can be generalized to implement adaptive search, an algorithm useful to optimization which cannot be implemented efficiently on classical machines. Combining Grover adaptive search with quantum encoding techniques, it may be possible to provide better than quadratic speedup in optimizing some families of scheduling problems.

Scheduling algorithms attempt to solve “scheduling problems”, which consist of finding the optimal order and distribution of a set of tasks on a set of machines or other resources. Classically, this class of problem is NP-hard, meaning that it cannot be solved in polynomial time, and practical algorithms to the problem set typically provide a “good” solution rather than the optimal solution [lu]. Application of Grover's quantum search [grover] to these problems typically still cannot produce polynomial-time algorithms; however, it can provide improved exponential-time algorithms that are more efficient than classical solutions. For example, the algorithm proposed in [lu] claims to return a schedule for running N jobs on M non-homogeneous machines as well as the longest job runtime in $O(\sqrt{M^N})$ time. This problem is known as the $R||C_{max}$ problem, and classically requires $O(M^N)$ time to solve. Lu and Marinescu describe in [lu] a systematic approach to reformulating other scheduling problems so that they can take advantage of Grover's search.

Scheduling problems emerge in a wide variety of scenarios. One example is in operating system design, where computer resources must be allocated for multiple jobs on a system. Another example is dividing tasks among workers in a business. Employees have varied abilities, and some are suited better to a certain type of job than others. Scheduling algorithms can help managers decide who should be working on what and when. The transportation industry faces a variety of scheduling problems, which include the additional complexity of requiring airplanes, trains, and trucks to follow connected routes. As quantum computers become commercially viable, quantum scheduling algorithms can be used to solve practical scheduling problems which are very difficult and time consuming to solve classically.

Before discussing adaptive search, we describe some necessary background on Grover's search algorithm [grover, grover1, grover2, kaye, nielsen]. Grover's search is an algorithm to search an unordered database. This problem is like trying to search a phone book to find which name corresponds to a phone number. Since there is no structural information to narrow down the search, classically each entry in the phone book must be checked sequentially to see if the associated entry matches the queried number. In the average case, the algorithm will search half of the entries before finding the target. In the worst case, there is no target (the number belongs to someone not in the phone book), and the algorithm searches the whole database before returning. Grover's algorithm takes advantage of a quantum computer's ability to manipulate a superposition of input states simultaneously and can find the target entry in $O(\sqrt{N})$ "lookups", where N is the number of elements in the database. The notion of a lookup (oracle function query) is slightly different between the quantum mechanical and the classical techniques since the quantum algorithm can "check" all of the input states at once. In some cases, there may be multiple target states in the database, and a successful search would return any of these states.

The first step of the algorithm is to initialize the system to an equal superposition of all input states. Typically, N is assumed to be a power of 2, so $N = 2^n$. Since memory is usually available in powers of 2, this assumption simplifies the algorithm because it does not need to account for unused states.

Next, the “Grover gate” is applied [$\pi\sqrt{N}$}/4] times. The Grover gate is made of two main components, a selective phase shift U_f and an “inversion about average” function U_ψ. The selective phase shift rotates the target states by π, essentially inverting their probability amplitudes. This function is known as the “oracle” function, which is the quantum equivalent of the “lookup” function. Unlike the classical version, it does not directly indicate what a target value is, but merely affects the probability amplitude of the target states. The inversion about average operation reflects the probability amplitude of each state about the average amplitude. These two operations increase the amplitude of the target state and reduce the probability of all other states. Since the probability of measuring a particular value is the corresponding state's amplitude squared, when a measurement is performed, a target value will be observed with probability greater than 1/2. Grover's search does not return a target state with probability 1, but if it is performed more than once, the probability that the result returned is a target state is increased. The returned result could also be checked classically to verify correctness, although this confirmation is not applicable in all cases.

While the number of Grover iterations required to maximize the amplitude of the target state(s) is less than $O(\sqrt{N})$, the amplitude fluctuates significantly based on the number of iterations and the proportion of the states that are marked. The probability of finding a target state is given by:

$$g_r(p) = \sin^2[(2r + 1)\arcsin(\sqrt{p})] \quad (5)$$

where p is the fraction of states that are marked and r is the number of applications of the Grover gate [baritompa]. A plot of $g_6(p)$ is shown in Figure 3. Depending on the value of p, 6 applications of the Grover gate could be successful with either very high, or very low probability. If the ratio p was known, one could easily determine the best number of iterations to apply, but p is typically unknown.

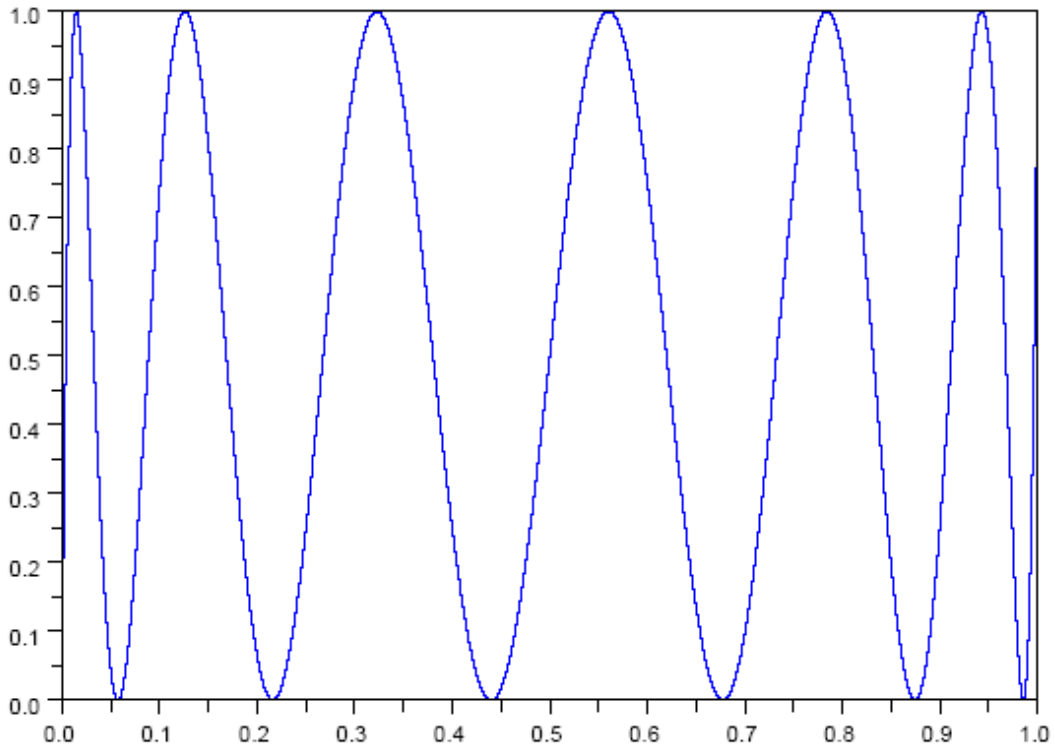


Figure 3. The probability distribution of observing a target state after 6 applications of the Grover gate with the fraction p of target states. Depending on the value of p, the search success probability varies greatly.

3.4.1 Adaptive Search

Adaptive search is an algorithm for finding the minimum value of f(x) for a finite set of values $x \in X$ by selecting decreasing values f(x) until the minimum is reached. The algorithm is as follows [bulger]:

x = random element of X
y = f(x)
FOR {i = 1,2... while $f(x_i)$ is not the minimum of f(x) for $x \in X$}
  $X_i = \{x \in X \mid f(x) < y_i\}$
  x' = random element of X_i
  y' = f(x')
  x_{i+1} = x' and y_{i+1} = y'
ENDFOR
return x'

There are two major problems with implementing this algorithm classically. First, the terminating condition is that $f(x_i)$ is not the minimum, meaning that in order to find value, x, that minimizes f(x), the minimum of f(x) must already be known. Second, identifying the set X_i, known as the improving region, classically requires checking each element of the previous improving region, negating any potential speedup of adaptive search. Grover's search, however, provides remedies for both of these flaws.

A quantum algorithm to find the minimum of a finite set was first proposed by Durr and Hoyer in [durr]. They proposed replacing the stopping condition by a time limit restraint. According to their analysis, after running for $22.5\sqrt{N} + 1.4\log^2 N$ units of time, their algorithm would return the minimum value with probability of greater than 1/2. Baritompa et al. determined that this result had incorrect constants, but was correct in order of magnitude, providing more rigorous analysis considering other parameters of the search [baritompa].

The second problem is solved naturally using the Grover operator. Using the oracle function, h(w) = (f(w) < Y), the target states are exactly the states in the improving region. A successful application of Grover search with this oracle function will return a random element from the improving region with uniform distribution. As x_i becomes increasingly close to the optimal value, however, the improving region shrinks and more Grover iterations are potentially required for the search to be successful.

Grover's search introduces a new complication to adaptive search due to the probability distribution defined by $g_r(p)$. Each successful iteration of adaptive search will decrease the fraction p, having a potentially dramatic effect on the probability of search success. If the number of applications of the Grover gate does not change between iterations, it is possible to stall at a point of low success probability, the minima of Figure 3. Varying the value of r can potentially avoid this problem and several methods of "rotation scheduling" have been proposed. The first is to select a random value between 0 and m where m is initially 1, and is multiplied by a factor λ after each failed search attempt [baritompa]. This approach has the advantage of being simple to compute, but m grows exponentially with the number of failures. Baritompa et al. propose a predefined sequence of rotations based on an estimate of p after each iteration. This sequence of r values performs slightly better in some cases, but computing the sequence requires exponential time and this sequence performs equally well with the randomized sequence when there are repeated values in the range in the search domain. Neither approach guarantees search success as p approaches 1/N.

Adaptive search has several important properties for optimization. First, unlike many classical minimization algorithms, adaptive search is not affected by local minima. Since the improving region is defined by the range of the function, not the domain, the global minimum will never be excluded from the improving region. Second, while most of the work done by the Grover implementation of adaptive search is done during the final iteration when the improving region is as small as possible, the intermediate results are generally good approximations of the minimum, especially if there are multiple values only slightly greater than the global minimum.

3.4.2 Framing Optimization Problems as Search Problems

The concept of quantum parallelism makes it possible to treat an optimization problem as a search problem with far fewer resources than are classically required. Classically, a brute force approach to optimization would be to test the set of all possible outcomes of the system being optimized (the state space of the system). Since the state space typically grows exponentially in size as systems become more complex, searching the entirety of the state space is usually computationally intractable. To overcome this, pruning is typically applied to reduce the size of the state space by excluding clearly non optimal or duplicate results. Correct and effective pruning requires knowledge of attributes and symmetries of the system that are often either unknown, or may not exist.

Classically, each state in the state space must be computed separately, either sequentially, or with a low level of parallellization. In a quantum computer, however, the entire statespace can be computed in a superposition with one operation. Once the state space has been prepared, algorithms like Grover adaptive search can be applied to determine the optimum solution.

Lu and Marinescu propose in [lu] a procedure for generating the state space for the R || C_{max} problem, which appears to be easily adaptable to other optimization situations. The quantum circuit described makes use of the entanglement between qubits by using controlled gates triggered by a set of index qubits. A circuit computing the state $|i\rangle|G_i\rangle$ is shown in Figure 4. If the input to the index qubits is an equal superposition of states, which can easily be prepared with Hadamard gates, and if all the necessary gates can be implemented efficiently, circuits like this can be chained together to create an equal superposition of all states in the state space.

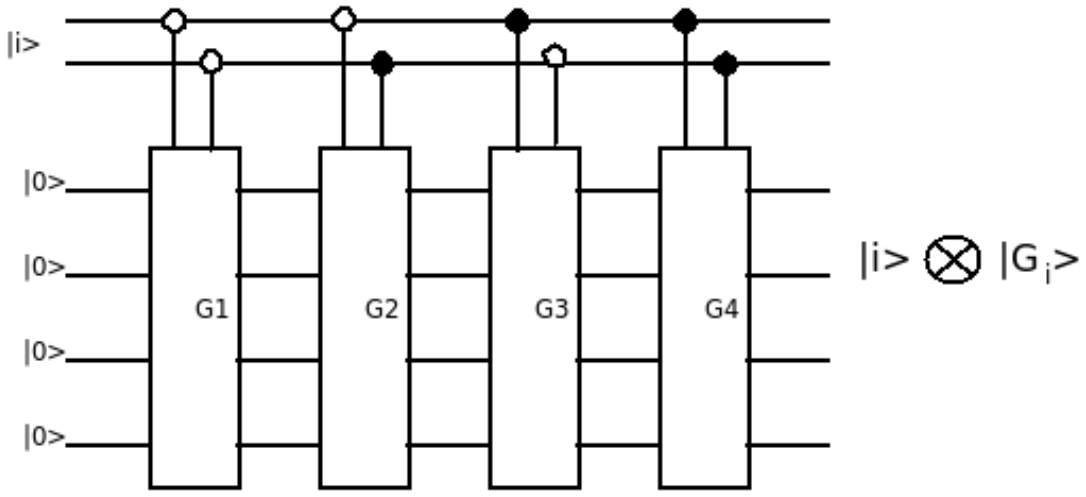


Figure 4. A quantum circuit computing the state $|i\rangle|G_i\rangle$. The index lines ensure that the gates G_i are each applied only once.

3.4.3 Using Grover Search to Find the Minimum

Once the state space has been computed, Grover adaptive search can be used to find the minimum or maximum of a particular parameter encoded in the superposition. Using an oracle function h(w) defined as h(w) = (f(w) < Y) where Y is an adjustable threshold value and w is the set of qubits of interest, an adaptive search like the one described in [baritompa] can be used to find the optimal value. The encoding described by Lu and Marinescu entangles the input states with the output states, so when a measurement is finally performed, the input states collapse into the set of inputs producing the measured output. This algorithm returns not only the optimal output value, but how to achieve it. Using a different encoding circuit or oracle function would produce a circuit that could minimize or maximize a variety of parameters of a system.

3.4.4 Results: Adaptive search simulation

In order to analyze the properties of adaptive search, several simulations were developed using classical techniques. These simulations verified the desirable properties of adaptive search. For example, the 1D function shown in Figure 5 demonstrates that the algorithm is not affected by local minima. Also, after a small number of iterations, all subsequent values are within a small range of the optimal value, even though they are in disconnected parts of the domain.

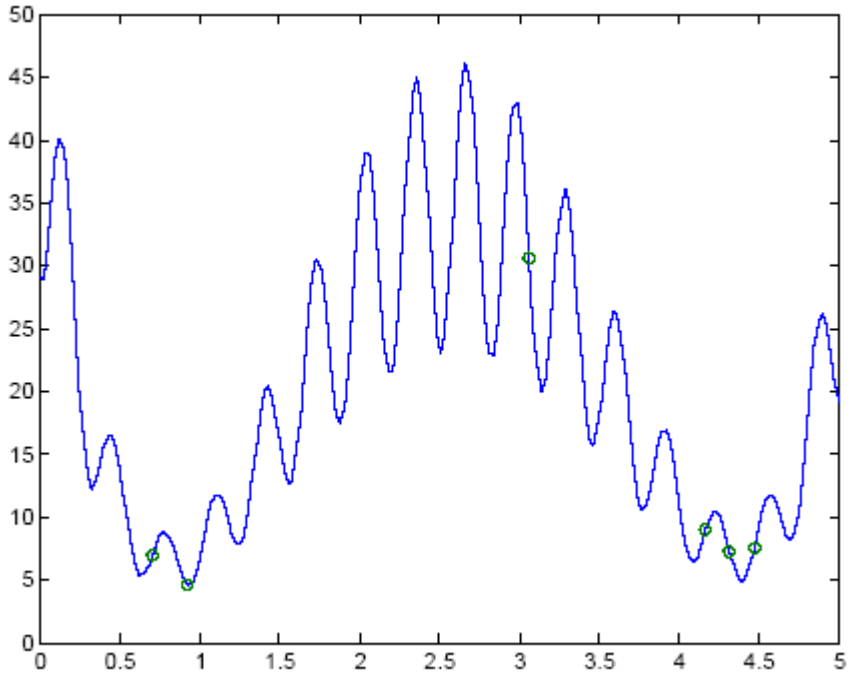


Figure 5. Successive iterations of adaptive search (circles) on a 1D function (solid line) with multiple local minima. The search converges quickly to the optimum value despite local extrema.

Extending this simulation to a 2D function already begins to demonstrate the limits of *classical* implementations of adaptive search. Since the domain grows exponentially in the number of dimensions, each additional dimension requires exponentially more resources to find the optimal value. However, in 2 dimensions, the same properties hold, as shown in Figure 6 and Figure 7.

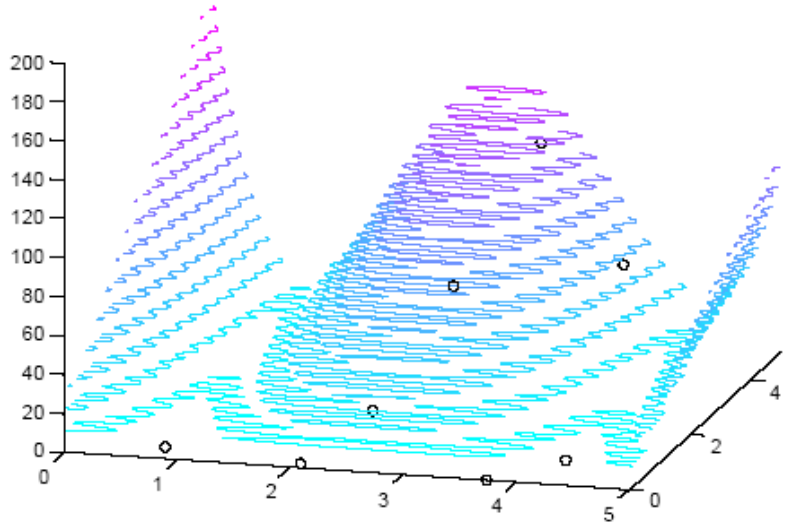


Figure 6. A 3D contour plot of a 2D function with successive adaptive search iterates. 2D adaptive search exhibits the same desirable properties as the 1D variant.

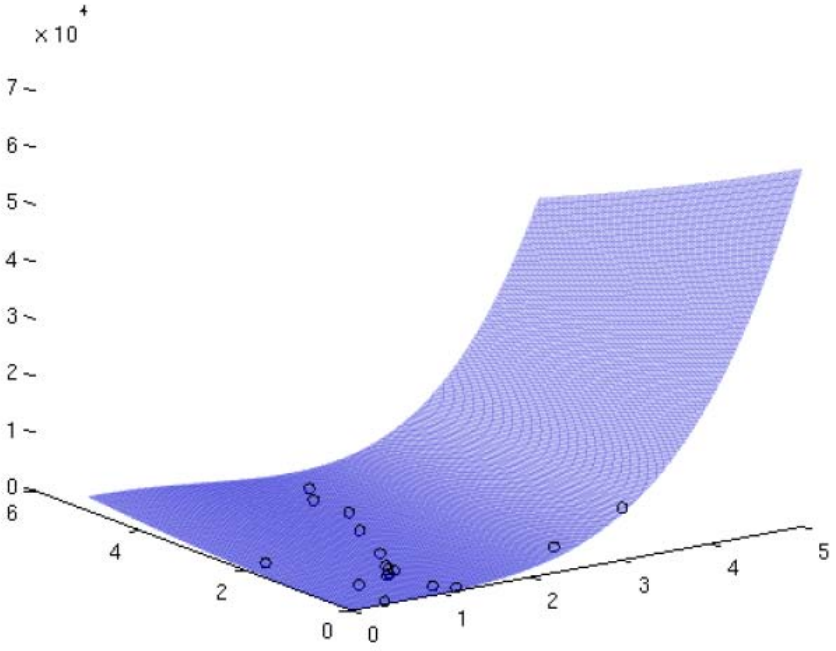


Figure 7. Adaptive search applied to the Rosenbrock banana function, a standard optimization objective function [bananaFunc].

3.4.5 Rotation Schedule Implementation

Baritompa et al. provide in [baritompa] an algorithm for computing a sequence of rotation counts to improve the probability of success of sequential adaptive search iterations. The algorithm requires indefinite integration of successive, increasingly complicated functions, which are not easily integrated. One way to actually compute these integrals is to represent the function $g_r(p)$ as a polynomial. The algorithm to generate the rotation schedule was implemented using a Taylor series approximation to $g_r(p)$ as well as an exact polynomial representation based on the Gauss hypergeometric function ${}_2F_1$,

$$g_r(p) = (2r+1)^2 \, p \, {}_2F_1^2\left(r+1, -r; \frac{3}{2}; p\right). \tag{6}$$

Examples are $g_1(p) = (3 - 4p)^2 p = 9p - 24p^2 + 16p^3$ and $g_2(p) = p[5 + 4p(4p - 5)]^2$. The degree of the terminating ${}_2F_1$ function in Equation 6 is r, so that the overall degree of $g_r(p)$ in p is 2r + 1. Due to the oscillatory nature of $g_r(p)$, shown in Figure 3, a very high order Taylor polynomial is required as r grows, rendering this approach infeasible at sufficiently large r. The hypergeometric function-based approach does not suffer from this problem, but as the integrals become increasingly complex, the computation time increases dramatically. With computational resources readily available (desktop PC), the hypergeometric function implementation was able to compute the first 30 terms of the rotation schedule in 24 hours in Mathematica. A plot of the first 30 terms of the sequence is shown in Figure 8.

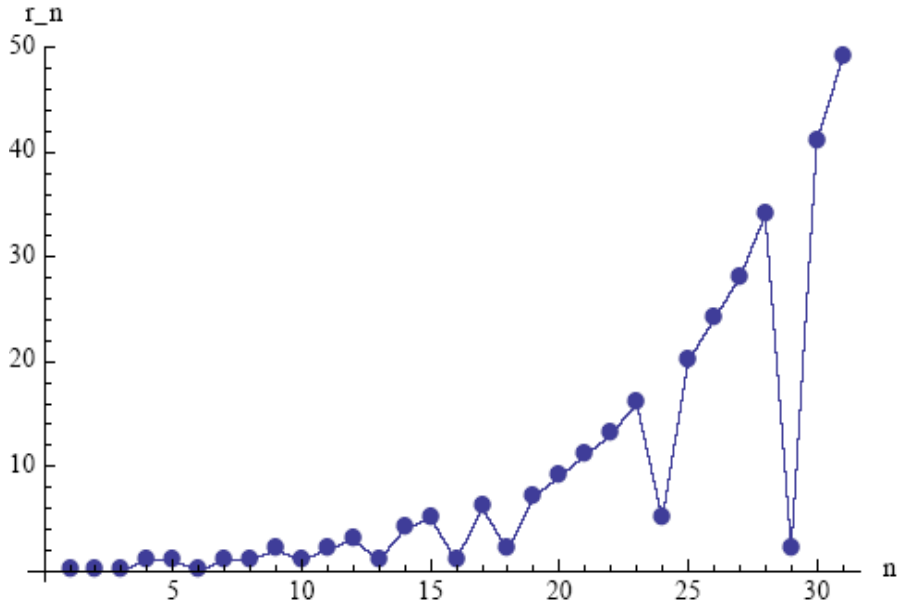


Figure 8. The first 30 terms of the rotation schedule described by [baritompa].

3.4.6 Future Work

3.4.6.1 Adaptive Search

The usefulness of Grover adaptive search hinges on the hypothesis that an oracle function like h(w) = (f(w) < Y) can be implemented efficiently. More research is required to design and efficiently implement a quantum circuit that can implement comparison operators such as “greater than” or “less than”.' This gate must be able to take two inputs because the threshold value Y will change with each iteration, so a hard coded value will not suffice. It remains an open question just how efficiently the needed oracles for generic problems may be implemented.

Baritompa et al. analyzed the Grover adaptive search algorithm to determine the expected number of iterations before finding the optimal value [baritompa]. However, a bound on how close to the optimal value can be expected after a number of iterations would be valuable as well. For example, if the second most optimal value can be found in half the time required to find the optimal value, it may be unnecessary to perform as many iterations.

3.4.6.2 Scheduling Problem Encoding

The encoding system developed in [lu] appears to be valid, however, there are a number of extensions that would likely be required in practice. The circuit as is requires that all inputs be integers. This is not a limitation in practice, since the least common multiple of all necessarily rational input parameters may be used.

3.4.6.3 Termination of the algorithm

Setting a run time bound on the size of the improving region to the total domain is a working possibility for a criterion for terminating the algorithm. However, many common global minima could be problematic. We may note that even in the easier “find Min” situation of Durr and Hoyer there is an interrupt on run time. The main question is again how well this can be done for generic problems.

3.4.6.4 Combining encoding and search

Once the quantum encoding of a scheduling problem is shown to be correct, and adaptive search has been shown to be as efficient as predicted, the two must be combined. In order to show that scheduling problems can actually be solved using this technique, the whole system must be simulated and benchmarked. The number of quantum gates required to construct these circuits could also be intractably large, so optimization of the circuit implementation may also be necessary to realize this algorithm.

3.4.6.5 Concluding thoughts on adaptive search

As quantum computers become closer to being viable, the development of quantum algorithms is becoming increasingly important. A quantum computer has the potential to solve problems such as scheduling problems that classically require prohibitive resources. Solutions to scheduling problems would have a broad reaching, positive impact on a variety of industries. Techniques exist to solve pieces of scheduling problems on a quantum computer: a quantum encoding of the problem, and an algorithm for optimization. By combining these techniques, it may be possible to solve scheduling problems that are intractable using classical techniques.

3.5 Feynman diagram integrals and special functions

Perturbative quantum field theory visually and systematically describes higher order corrections by means of Feynman diagrams. In many cases the corresponding multidimensional Feynman integrals may be reduced all the way to one dimension. In recent years both rigorously and empirically based expressions for these integrals in terms of values of special functions have appeared. In a series of articles, we have made a number of contributions for closed form results for reduced Feynman integrals [cofjmp1, cofjmp2, cj, cl, coffey08]. We were also able to advance the state of the art of the theory for particular special functions of mathematical physics, including the Clausen function Cl_2 and the dilogarithm function Li_2. Other specific special functions that were very useful included the generalized hypergeometric functions and the polylogarithms. Results to date indicate connections between multiple subjects including hyperbolic geometry, analytic number theory, special functions, and Feynman diagrams. A very recent example [cofjmp1] evaluates a highly symmetric Feynman integral in terms of a remarkably compact difference of Clausen function Cl_2 values, proving a numerically based conjecture that was open for approximately ten years.

A certain dilogarithmic integral I_7 turns up in a number of contexts including Feynman diagram calculations, volumes of tetrahedra in hyperbolic geometry, knot theory, and conjectured relations in analytic number theory. We provided an alternative explicit evaluation of a parameterized family of integrals containing this particular case. By invoking the Bloch-Wigner form of the dilogarithm function, we produced an equivalent result, giving a third evaluation of I_7. We also alternatively formulated some conjectures which we posed in terms of values of the specific Clausen function Cl_2 [cofjmp2, coffey08].

The evaluation of harmonic number sums has been useful in several areas of mathematics, including analytic number theory, for some time. More recently, the evaluation of Euler sums has been shown important in various areas of theoretical physics, including in support of Feynman diagram calculations. Even more recently, it has been shown that the evaluation of generalized harmonic number sums is very useful in resolving open questions on Feynman diagram contributions and relations among special functions [cofjmp1], including the dilogarithm, Clausen function, and generalized hypergeometric function. Harmonic number sums also occur in computer science in the efficiency analysis of algorithms. Especially in the analysis of sorting and searching algorithms, harmonic number sum evaluation and asymptotic analyses are useful.

Motivated by such applications, we have developed results on generalized harmonic number sums [cl]. We give results where evaluations are possible in terms of generic polylogarithm functions Li_k, although we give specializations to the dilogarithmic and trilogarithmic cases, where a fuller body of theory exists, and relatively more instances of explicit expression of specific values in terms of elementary functions is possible. We demonstrated the evaluation of a class of generalized harmonic number sums, presented examples, and then gave representative results for obtaining identities among harmonic number sums in terms of polylogarithmic functions.

As a result of these research activities, the PI was invited as a speaker at a very recent workshop dealing with Feynman diagrams, multiple zeta values, and integrals [workshop]. Other areas of mathematics covered in this workshop were abstract algebra, combinatorics, and graph theory. The main areas of theoretical physics concerned were quantum field theory and quantum statistical mechanics. The PI gave two lectures at the graduate level on Feynman diagrams, integration, and special functions.

3.6 QLGAs for the Maxwell equations

In our research we showed that a quantum lattice gas approach can provide a viable means for numerically solving the classical Maxwell equations. By casting the Maxwell equations in Dirac form, the propagator may be discretized, and we described [coffey] how the accuracy relative to the time step may be systematically increased. The quantum lattice gas form of the discretization is suitable for implementation on hybrid classical-quantum computers. In the published paper [coffey] we also discuss a number of extensions, including application to inhomogeneous media.

The analytic and numerical modeling of electromagnetic phenomena is a subject of much practical importance. Due to a panoply of ingredients including geometry, dimensionality, boundary, initial, and radiation conditions, and constitutive relations, nature presents a rich variety of these phenomena.

In this section we introduce the formulation of the Maxwell equations as quantum lattice gas algorithms. In this way, the partial differential equations of electromagnetism are discretized in both space and time, permitting numerical simulation. Here we concentrate on the theoretical framework, but we provide sufficient detail that software implementations could be developed. Many extensions of our approach are possible, and we described several of them elsewhere [coffey].

We exploit the formulation of the Maxwell equations for the electromagnetic field in terms of a multicomponent wave function, and this wave function need not correspond to a spin 1 particle. Auxiliary conditions are used as necessary to ensure that the full set of Maxwell equations is satisfied.

It has been known for some time that the Maxwell equations may be written in Dirac form [iwoprd, moses]. We complemented this framework, and provided supporting techniques so that competitive algorithms could be developed. Generally the Maxwell equations in the continuous setting may be brought into the form:

$$\partial_t \psi = \kappa \, S \bullet \nabla \psi, \qquad (7)$$

where κ is a constant, S_j are three spin matrices of suitable dimension, and ψ the corresponding wave function. We focused on ∇ as the three dimensional (3D) gradient operator, but this is by no means necessary. The result of discretizing Equation 7 is to present the time evolution of ψ in terms of spatial shift and spin-component mixing operations. In the language used in a very related setting, these operations may be rewritten as streaming and collision operations, respectively.

Having written a discretization of Equation 7, we take the further step of writing the discrete evolution operator in terms of a product of collision and streaming operators. It is this form of the discrete evolution that could be implemented on a hybrid processor, wherein local nodes of a few qubits are connected via classical communication channels to neighboring nodes. The on-site collision operator generates entanglement within the individual nodes. As it is unitary, it can be realized in a quantum system, and further provides a stable algorithm. In sum, our procedure shows how to discretize systems such as Equation 7 in a number of settings, and importantly in a factorized form suitable to combined classical-quantum computing.

Lattice gas algorithms have proved very efficient and versatile in a variety of contexts, including fluid dynamics and plasma physics and other multi-particle simulations [rothman, yepez, vahala]. They have been used to numerically solve the Navier Stokes and Boltzmann equations in diverse geometries, upon a range of computing platforms. A key feature of these algorithms is their suitability for parallel and distributed computing (e.g., [harting]). We point out that it should be possible to develop these same advantages for solving the Maxwell equations. Moreover, there are now prospects for nearer term hybrid classical-quantum computing (e.g., [pravia, berns, chen06]) as well as more distant purely quantum processors [nielsen]. Various quantum lattice gas algorithms have been proposed for the solution of the Dirac and Schroedinger equations [boghosian98, yepez02]. Further development of the types of algorithms that we suggest would allow the exploitation of entanglement in quantum hardware. This would be an additional resource, on top of the classical parallelization aspects of these algorithms.

Significant portions of our work made use of results of I. Bialynicki-Birula [iwoprd, iwoacta, iwohep], who was mainly interested in theoretical constructions. In [coffey] we recalled the formulation of the Maxwell equations in Dirac (spin 1/2) form, providing a self-contained development, which may make this subject accessible to a wider audience. We then considered a spin 1 formulation of the Maxwell equations and again took it as the basis of a computational method. For both formulations, we provided supporting details. We then described a number of extensions, including how to improve the convergence rate of the discretizations, this latter important topic applies to either the spin 1/2 or spin 1 formulations.

We have shown how the multicomponent wave equations of relativistic quantum mechanics may be adapted for a description and numerical solution of the classical Maxwell equations. Written in a spin 1 form, the wave function has three independent components that are directly applicable to describing the massless photon, whereas written in a spin 1/2 Dirac form, the four-component wave function requires a constraint condition. By discretizing the quantum evolution operator (propagator), we have derived algorithms for integrating the Maxwell equations. These algorithms provide an explicit numerical integrator and are suitable to any number of spatial dimensions. This approach contrasts with that of first discretizing the system Hamiltonian, which may often lead to physical and mathematical difficulties.

As seen in detail in [coffey], there are equivalences with effective finite difference approximations of the partial differential equations, and this is not surprising mathematically. However, physically our approach provides connections with the path integral formulation of quantum mechanics, and this was a motivating reason behind the work of [iwoprd]. Indeed, an iteration of a discretized time evolution gives a sum over Dirac particle histories.

We emphasize that mathematical equivalences are quite distinct from software and hardware implementations. Whereas, to be very specific, a finite difference representation is suitable for either serial or parallel processing, the lattice gas forms are also very suited to a parallel architecture. The lattice gas representation comprises two main stages. One is the local aspect, embodied in W or collision matrices C acting on local field or wave function components. The other is the advective (or streaming) stage shown by the shift operators moving field information to neighboring sites. Collections of lattice sites may be mapped to local computing nodes of minimal resources within a parallel machine. For instance, for a square lattice, blocks of rows or columns of the lattice may be mapped to individual processors, or instead checkerboard subblocks may be mapped to the processors. In this way, parallel computers with a large number of nodes but each with limited computing capability and memory may be taken advantage of, with many variations on these ideas possible.

There is no difficulty in increasing the rate of convergence of our family of algorithms. One has only to apply systematic Trotter-Suzuki formulas [suzuki] for improved discretization of the propagator.

We have briefly given an extension of the lattice gas approach to inhomogeneous media, and expect that other extensions are possible [coffey]. Already in one or two dimensions, this opens the way for solving a variety of interesting and practical problems.

While we have focused on the Maxwell equations, many other applications could be developed when the systems of governing partial differential equations can be cast in the form of Equation 7, and this point furthers the argument for the very wide applicability of lattice gas algorithms. One example extended coupled system is the Maxwell-Schroedinger equations. Here the absolute square of the wave function ψ^2 and $\psi^*\nabla\psi - \psi\nabla\psi^*$ feed into the charge and current densities, respectively. Another example coupled system is the Maxwell-London equations for a phenomenological description of superconductivity, wherein the London relation links the vector potential to the supercurrent density.

3.7 Telegraph Equation QLGA

The telegraph equation combines features of both the diffusion and wave equations and has many applications to heat propagation, transport in disordered media, image enhancement, and elsewhere. In this section we give an overview of a new quantum lattice gas algorithm for this partial differential equation with one spatial dimension. This algorithm generalizes one previously known for the diffusion equation. In [cc2009] we present many further details, including an analysis of the algorithm and accompanying simulation results. The QLGA is suitable for simulation on combined classical-quantum computers.

Quantum lattice gas algorithms are well known to be versatile in simulating a wide range of physical phenenomena. Like their relatives cellular automata, from simple local rules, complex dynamics may emerge [brennen, romanelli].

Lattice gas algorithms are attractive due to their relative simplicity, physical foundations, and suitability for implementation on parallel computing architectures. Lattice gas algorithms may incorporate conservation of mass, momentum, and energy, and in the quantum context, probability. Lattice gas algorithms have proven successful in a range of applications including fluid dynamics and plasma physics and other multi-particle simulations [doolen, rothman, yepez].

Recent experiments and proposals for combined classical-quantum computing (e.g., [berns, chen06, pravia]) further motivate the development of quantum lattice gas methods. For instance, a QLGA for the linear diffusion equation has been demonstrated in a liquid-state nuclear magnetic resonance system [pravia]. In addition, a detailed design for executing a QLGA for the linear diffusion equation with superconducting qubits has been given [berns]. Such implementations could allow the exploitation of quantum entanglement well before large-scale purely quantum computers are constructed.

In this section we discuss a new QLGA for simulation of the telegraph equation. This hyperbolic partial differential equation combines aspects of both the wave and diffusion equations. As such, our algorithm subsumes some earlier work restricted to the diffusion equation. Representative numerical results verifying the algorithm and its analysis are published elsewhere [cc2009].

Classical connections between random walk and the telegraph equation have been known for quite some time [goldstein, kac, gaveau, morette, codling]. In such a model on a one-dimensional (1D) lattice, a walker steps a distance Δx in time increment τ randomly to the left or right, with additionally a probability $a\tau$ to reverse direction. In the simultaneous limit that $a \rightarrow \infty$ as well as the speed v, such that the ratio $2a/v^2 \equiv 1/D$ remains constant, the diffusion equation results,

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}. \tag{8}$$

Another situation for which this equation results is when $a\tau = 1/2$. Then there is equal probability for a move to the left or right. In a sense, we seek a quantum version of this stochastic model.

We also mention a connection of the telegraph equation with relativistic quantum mechanics and the point of view of a Dirac particle as moving at the speed of light c with random reversals of direction. If we write the telegraph equation in the form $(\partial_t^2-2a\partial_t-c^2\partial_x^2)P = 0$, then the change of dependent variable $P(x,t) = e^{-a\,t}\psi(x,t)$ shows that ψ satisfies the Klein-Gordon equation $(\partial_t^2-c^2\partial_x^2-a^2)\psi = 0$. Both the telegraph and Klein-Gordon equations may be factored into a pair of equations first order in time, with the latter instance giving the well known Dirac equation. In the case of a Dirac particle, we identify the frequency of probability of reversal $a = m_0c^2/ih'$, with m_0c^2 the rest mass energy [gaveau]. This can provide, for example, an interpretation for the Zitterbewegung phenomena of Dirac theory.

Classically or quantum mechanically, lattice gas dynamics may be thought of in terms of scattering due to local potentials. There is an associated scattering matrix, leading to transmission and reflection coefficients. Building upon such an approach, recent work has used quantum random walk to examine diffusion in 1D crystalline nanostructures [godoy]. The telegraph equation results in the continuum limit for an irreversible, *second-order* Markov process.

A QLGA includes the sequential repetition of four main steps [yepez, yepez01, yepez06, vahala]. First, initialization creates the quantum-mechanical initial state that corresponds to the intial probability distribution for a partial differential equation to be solved. Secondly, in the collision step, a unitary transformation is applied in parallel to all the local Hilbert spaces in the lattice. Next, in the measurement step, the quantum states of all the nodes are read out. Lastly, these results are shifted or "streamed" to neighboring lattices sites, providing reinitialization of the lattice in the state which corresponds to the updated probability distribution.

QLGAs have been shown to solve the diffusion, Burgers, Boltzmann, Schroedinger, and Dirac equations [yepez, vahala, yepez01, boghosian98, yepez02]. In some QLGAs (e.g., [boghosian98, yepez02]) the measurement step is omitted and the generally entangled quantum states are streamed. This places much stronger requirements on the quantum computing hardware, but gives an exponential speed up over classical simulation. We discuss an algorithm with intermediate-time measurements.

There is much applications interest in both classical and QLGAs. Elsewhere [coffeycolburn], we have demonstrated that hybrid computing, running versions of diffusion processing, could be useful for the enhancement of digital images. In particular, diffusion of intensities, with a constraint on the difference of pixel iterate values, gives selective smoothing within an image. In another very recent scenario, we have developed QLGAs for the Maxwell equations by starting from a Dirac formulation [coffey]. The algorithms may be executed with measurement only at the final time, resulting in an exponential speed up over classical simulation.

Very recently, a telegraph-diffusion operator has been proposed for purposes of image restoration and denoising [ratner]. This approach requires the solution of a nonlinear telegraph equation with diffusivity dependent upon the gradient of the intensity function. Our results now indicate the possibility to apply a QLGA with a signal strength constraint for a 1D telegraph equation for obtaining the denoising of digital signals.

A drawback of the ordinary diffusion Equation 8 for many applications is that the associated propagation speed is infinite. For any positive time t, there can be diffusion, albeit usually very small, to arbitrarily large distances. The telegraph equation offers one way of correcting this aspect: it models diffusion with a finite propagation speed. This can be very important for modeling diffusion in a variety of contexts including turbulent fluids and biological processes and ecological problems (e.g., [codling]). The search for a fully special relativistic diffusion equation remains an open and important problem for statistical physics and other areas, but the telegraph equation provides an improvement over Equation 8.

Whereas the parabolic Equation 8 has a number of well known properties, including satisfying a maximum principle, the behavior of solutions of the telegraph equation is generally more complicated. As shown for instance by a Fourier series solution of the telegraph equation with special zero Dirichlet or Neumann boundary conditions, there is a variety of behavior of the solutions of the telegraph equation.

The QLGA has a significant numerical advantage inherent in its formulation. This is the guaranteed stability due to the use of a unitary collision operator. For a hyperbolic equation as we are dealing with here, this is no small matter. We recall that in comparison an explicit finite difference scheme for a wave equation must satisfy the Courant-Friedrichs-Levy condition [gasdynbk] as a *necessary* constraint. Roughly described, the Courant-Friedrichs-Levy condition arises from ensuring that the domain of dependence of the numerical method contains the domain of dependence of the partial differential equation being solved. It has the direct consequence of limiting how large the time step may be taken in relation to the size of the spatial discretization. The severity of the Courant-Friedrichs-Levy condition can be reduced only at substantial computational cost. Either the time step is drastically reduced, or another method such as an implicit scheme is required. In the latter event, there is significant additional computational cost in solving a set of coupled equations at each time iteration. Even then, if the boundary conditions are not treated fully implicitly also, the Courant-Friedrichs-Levy constraint will become manifest.

A QLGA also offers a significant advantage as far as realizing a hybrid architecture. This is because if the nodal qubits have sufficiently long coherence time, no quantum error correction is required. In contrast, many other methods require quantum error correction, and this is typically a tremendous increase in resource. Typical error correcting techniques encode one logical qubit in either 5 or 7 physical qubits. On top of this, several levels of concatenation are used.

The 1D telegraph equation arises as the probability density function (pdf) for the displacement at time t for persistent random walk on a 1D lattice in the continuum limit. With a form of momentum introduced into the random walk, persistent random walk has applications in describing scattering and diffusion in disordered media. As we have mentioned, the telegraph equation has solutions with a finite velocity of propagation, and this can provide an advantage for describing heat propagation, light dispersion in turbid media, or in biological modeling.

We have discussed a new QLGA for the 1D telegraph equation that subsumes one for the diffusion equation, while complementing that for the 1D Dirac equation. Both the telegraph and Dirac equations may be developed from microscopic models with particles undergoing random reversals of direction. The resulting QLGA for the 1D telegraph equation is highly parallelizable and well founded on physical principles including conservation laws. This algorithm offers the prospect for simulation on combined classical-quantum computing architectures. In such a computing environment, local nodes with two qubits each are connected to nearest neighbors with classical communication.

We have verified our QLGA on model problems which take into account the boundary conditions and the initial conditions on both the solution and its first order time derivative [cc2009]. Test problems included those from references [goldstein] and [morette]. Despite using an approximation to implement non periodic boundary conditions for some test problems, we were still able to find accurate solutions. The incorporation of further types of boundary conditions is an area for future research.

4. Summary

The concepts of entropy and of diffusion have been common themes throughout much of this research. Diffusion and the accompanying idea of scale space find many applications in image sharpening and restoration and other processing tasks. Entropy measures provide a useful monitor of diffusion processing, as well as a way to understand the information content of images.

In the overall scope of the investigations, we were able to make contributions to quantum information science over a fairly broad range of topics, from a new high level algorithm to detailed logic gate decompositions. The vast majority of these topics are additionally complemented with external publications.

As a byproduct, we made various contributions to the analytic evaluation of reduced Feynman diagram integrals. In doing so we advanced the theory of some particular special functions of mathematical physics and elaborated the theory of generalized harmonic number sums.

We found often that much 'ground work' needs to be done—there is an absence of quantum algorithmic 'infrastructure'. Although quantum computing is a very active area, just which applications are most amenable to quantum approaches often remain elusive. Two example questions from the latter portion of our overall investigation include: Which scheduling and logistics problems have oracle functions that may be implemented efficiently in order to perform adaptive search? Which type of limited logistics problem may yet have a polynomial-time quantum solution?

Lastly we made specific contributions to quantum lattice gas algorithms. We showed how the important Maxwell equations of electromagnetism could be solved with this class of algorithms. We further generalized an algorithm for the diffusion equation so that the more complicated telegraph equation could be simulated with a QLGA. The latter partial differential equation has multiple applications, including transport in disordered media, image enhancement, heat propagation, and elsewhere.

As a result of this project, senior student Ben James Jones received the Ryan Sayers memorial award for research as a combined computer science and engineering physics major.

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6. List of Acronyms

CNOT – controlled-NOT
PDEs – partial differential equations
QLGAs – quantum lattice gas algorithms

7. Appendix: Publications

The following articles, published or currently under review, were at least partially supported by the research contract.

M. W. Coffey and G. G. Colburn, Proc. Royal Soc. A **463**, 2241 (2007).

M. W. Coffey and G. G. Colburn, Phys. Rev. E **79**, 066707 (2009).

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